

# Optothermal transfer simulation in laser-irradiated human dentin

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## 1 Introduction

Laser technology has become an important tool used in several applications in dentistry including hard tissue ablation, oral surgeries, laser therapy, and reduction of dentinal hypersensitivity symptoms. Based on the temperature increase on the surface, Nd:YAG laser ( $\lambda = 1064$  nm) irradiation in dentin causes surface melting that can mechanically block the dentinal tubules.<sup>1–6</sup> The resulting molten layer can avoid the movement of the liquid contained inside the dentinal tubules, which is the largely responsible for the dentin hypersensitivity symptoms.<sup>1</sup> Thus, the major concern during laser irradiation of teeth is the high potential of tissue overheating resulting in high temperatures that can spread in toward the dentin, causing irreversible damage to cells present in the pulp chamber and leading to cell death.

During laser irradiation, the final temperature for any tissue will be dependent mainly on its absorption properties at a determined wavelength.<sup>7</sup> Thermal damage induced by laser radiation seems to be a tradeoff between thermal and mechanical damage in surrounding tissues,<sup>8</sup> where the first phenomenon seems to be more evident in dentin, as seen by the morphological effects after Nd:YAG laser irradiation on dentin surface.<sup>2–4</sup> These optothermal alterations in surface morphology can be enhanced when longer laser pulses containing high energy are used.<sup>8</sup> Hence, shortening the laser pulse width ( $\tau_p$ ) can reduce damage on dental pulp caused by temperature rise in surface during laser radiation. The use of pulsed laser radiation, as opposed to a continuous one, is advantageous due to: 1. the possibility of achieving precise cutting control and minimize the zone of thermal damage by producing a thermal event that is shorter than the thermal conduction re-

**Abstract.** Laser technology has been studied as a potential replacement to the conventional dental drill. However, to prevent pulpal cell damage, information related to the safety parameters using high-power lasers in oral mineralized tissues is needed. In this study, the heat distribution profiles at the surface and subsurface regions of human dentine samples irradiated with a Nd:YAG laser were simulated using Crank-Nicolson's finite difference method for different laser energies and pulse durations. Heat distribution throughout the dentin layer, from the external dentin surface to the pulp chamber wall, were calculated in each case, to investigate the details of pulsed laser-hard dental tissue interactions. The results showed that the final temperature at the pulp chamber wall and at the dentin surface are strongly dependent on the pulse duration, exposure time, and the energy contained in each pulse. © 2003 Society of Photo-Optical Instrumentation Engineers. [DOI: 10.1117/1.1560000]

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laxation time ( $\tau_r$ ) of the tissue; See eq. (7) below. 2. the delivery of sufficient energy in each pulse to ablate or modify the tissue, removing hot tissue before heat is transferred to the adjacent structures; and 3. ablation of dense tissue such as bone or tooth by rapid heating and/or plasma formation.<sup>8</sup>

Several studies have shown the effects of laser irradiation on dental pulp, but the results are controversial. Some reports demonstrated no effect on pulp, while others reported different levels of damage. Powell, Whisenant, and Morton<sup>9</sup> demonstrated that a temperature rise of 6 °C can cause irreversible pulp damage, and temperature rise of 11 °C may cause pulp cell death by apoptosis.<sup>10</sup> It is worth noting that there is some confusion in the literature about thermal effects associated with Nd:YAG laser irradiation on dentin, due to the variety of the laser parameters used.

The use of a Nd:YAG laser to promote dentinal sealing as a dentinal hypersensitivity treatment offers a series of advantages when compared to a CO<sub>2</sub> laser emitting at 10.6  $\mu\text{m}$ . For instance, dentin irradiation using a CO<sub>2</sub> laser can produce more extensive cracking lines than a Nd:YAG laser,<sup>11</sup> mainly attributed to the carbonization and subsequent contraction of the tissue due to loss of the collagen matrix during laser irradiation<sup>12</sup> and carbonization on the dentin surface. However, some studies have shown that radiation in the range of 9.3 to 9.6  $\mu\text{m}$  is strongly absorbed by dental hydroxyapatite,<sup>13</sup> thus, less energy might be required to produce surface changes.

This work simulates the temperature distribution in dentine during Nd:YAG laser irradiation of dentine surface using the

**Table 1** Summary of the sample groups and their irradiation parameters.

Group	Energy per Pulse	Number of Pulses	$\tau_p$	Pulse Interval
Group 1	900 mJ	1	0.9 ms	Single pulse
Group 2	450 mJ	2	0.9 ms	300 ms
Group 3	300 mJ	3	0.9 ms	300 ms
Group 4	150 mJ	6	0.9 ms	300 ms
Group 5	900 mJ	1	90 ms	Single pulse
Group 6	450 mJ	2	90 ms	300 ms
Group 7	300 mJ	3	90 ms	300 ms
Group 8	150 mJ	6	90 ms	300 ms

Crank-Nicolson’s numerical finite difference scheme,<sup>14</sup> and presents a brief discussion of the relevant photothermal mechanisms.

## 2 Parameters and Methods

### 2.1 Laser Parameters

The laser parameters used to calculate the optothermal behavior throughout dentin are described in Table 1. They were selected from our previous studies, where the dentin phase transition threshold was determined by varying the pulse width with a pulse interval of 300 ms. This threshold was achieved using an energy density of 180 J/cm<sup>2</sup> and laser beam diameter of 0.8 mm, corresponding to the total energy density for the eight different irradiation regimes described in Table 1. The morphological changes in the dentin surface resulting from Nd:YAG laser radiation will be described elsewhere.

### 2.2 Heat Transport Simulation

The finite difference method is based on the substitution of derivatives in the governing equation, resulting in a set of algebraic equations, which can then be solved if initial boundary conditions are known. Thus, the temperature can be calculated for each point; however, the numerical solution is always an approximate one, which depends on the specific numerical formula, its stability, and convergence. The Crank-Nicolson technique offers an unconditionally convergent solution for the heat conduction equation. In the present study, this method was used to simulate the temperature at the dentin surface and the heat diffusion toward the pulp chamber after Nd:YAG laser radiation using a one-dimensional formulation and constant thermal and optical parameters described by Seka et al.<sup>15</sup> (see Table 2).<sup>16,17</sup> Although the radial beam dimension is not much larger than the penetration depth of a Nd:YAG laser, the one-dimensional approximation can be still valid for the sample thickness and the beam spot of interest, used in this simulation.<sup>15</sup>

The Crank-Nicolson method is unconditionally stable, even for arbitrarily large time steps. This is advantageous for many applications, because the stability of this scheme means that the errors diminish rather than grow with the time.

The thermal distribution in dentine submitted to laser radiation can be described by the one-dimensional heat conduction equation:<sup>12</sup>

$$\rho c \frac{\partial T(x,t)}{\partial t} = k \frac{\partial^2 T(x,t)}{\partial x^2} + Q(x,t), \quad (1)$$

where  $\rho$  is the mass density (g cm<sup>-3</sup>),  $c$  is the specific heat (J g<sup>-1</sup>°C<sup>-1</sup>),  $T$  is the temperature (°C),  $t$  is the time (s),  $k$  is the thermal conductivity (W cm<sup>-1</sup>°C<sup>-1</sup>),  $x$  is the coordinate perpendicular to the surface (cm), and  $Q$  is the heat source, which can be calculated from the one-dimensional optical diffusion solution:

$$Q(x,t) = \mu_a I_o(t) \exp(-\mu_{\text{eff}} x) \quad (2)$$

where  $\mu_a$  is the absorption coefficient (cm<sup>-1</sup>),  $I_o$  is the incident intensity (W cm<sup>-2</sup>), and  $\mu_{\text{eff}}$  is the effective attenuation coefficient defined as:

$$\mu_{\text{eff}} = \{3\mu_a[\mu_a + (1-g)\mu_s]\}^{1/2}, \quad (3)$$

where  $g$  is the anisotropy parameter and  $\mu_s$  is the scattering coefficient (cm<sup>-1</sup>).

The spatial differentials are approximated by central difference and the temporal differentials are approximated by backward difference in time as follows<sup>18</sup>:

**Table 2** Thermal and optical constants of dentin ( $\lambda=1054$  nm).

Density ( $\rho$ ) <sup>16</sup>	2.1 gcm <sup>-3</sup>
Specific heat ( $c$ ) <sup>16</sup>	1.17 Jg <sup>-1</sup> °C <sup>-1</sup> ,
Thermal conductivity ( $\kappa$ ) <sup>16</sup>	6.3 × 10 <sup>-3</sup> Wcm <sup>-1</sup> °C <sup>-1</sup> ,
Scattering coefficient ( $\mu_s$ ) <sup>17</sup>	260 cm <sup>-1</sup>
Absorption coefficient ( $\mu_a$ ) <sup>17</sup>	3 cm <sup>-1</sup>
Anisotropy parameter <sup>17</sup>	0.93

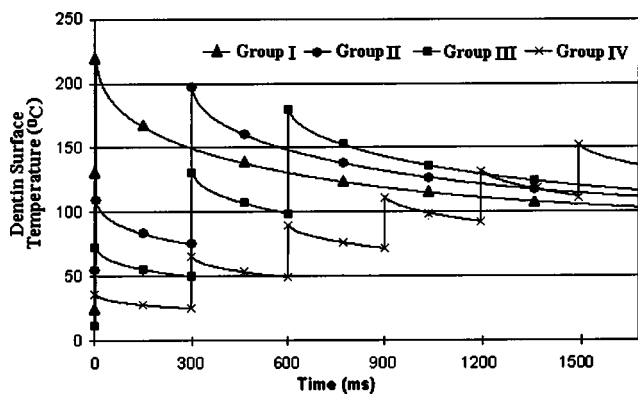


Fig. 1 Temporal evolution of the temperature at dentin surface during laser radiation with 1, 2, 3, and 6 pulses ( $\tau_p=0.9$  ms).

$$\left(\frac{\partial^2 T}{\partial x^2}\right)_i^{h+1} = \frac{T_{i+1}^{h+1} - 2T_i^{h+1} + T_{i-1}^{h+1}}{\Delta x^2}, \quad (4)$$

$$\left(\frac{\partial T}{\partial t}\right)_i^{h+1} = \frac{T_i^{h+1} - T_i^h}{\Delta t}, \quad (5)$$

where  $i$  is the space node and  $h$  is the time.

The resulting system of tridiagonal finite difference equations can be expressed in a compact matrix form as:

$$(I - \frac{1}{2}\ell A)T^{h+1} = (I + \frac{1}{2}\ell A)T^h + \Delta t D, \quad (6)$$

where  $T$  is the temperature vector  $\ell = \Delta t/\Delta x^2$ ,  $I$  is the identity matrix,  $A$  is a tridiagonal matrix and  $D$  is the boundary conditions.

The system of Eq. (6) can be solved directly by the application of the tridiagonal algorithm.<sup>19</sup> In this study, the compact form was used.

### 3 Results

The results of the optothermal simulation are shown in Figs. 1–4. The simulated evolution of temperature at the surface during laser irradiation using 0.9 and 90 ms pulses are presented in Figs. 1 and 2, respectively, where we observe that as the number of pulses increases, the amplitude of the rise of

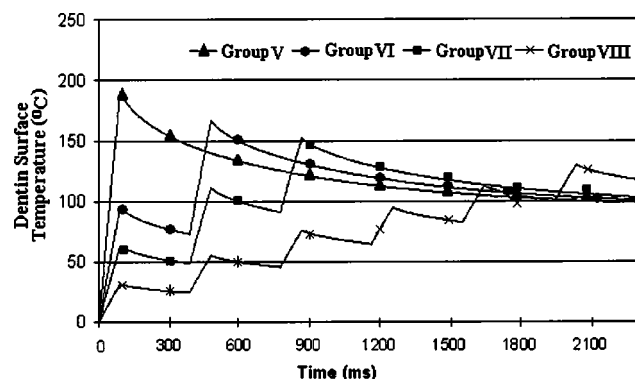


Fig. 2 Temporal evolution of the temperature at dentin surface during laser radiation with 1, 2, 3, and 6 pulses ( $\tau_p=90$  ms).

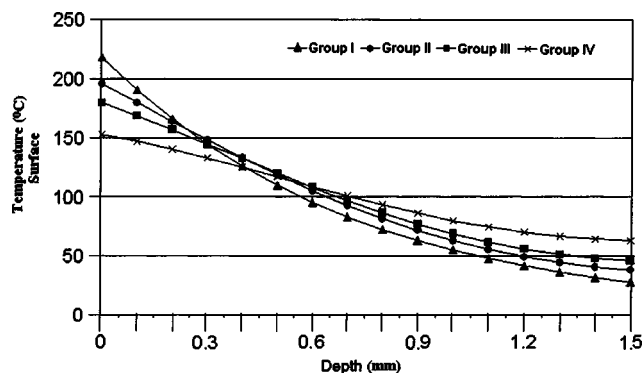


Fig. 3 Spatial temperature distribution for 1, 2, 3, and 6 pulses immediately after the end of the last laser pulse ( $\tau_p=0.9$  ms).

temperature in surface decreases. The highest temperature rise ( $\sim 218^\circ\text{C}$ ) was resulted from a single pulse irradiation with  $\tau_p=0.9$  ms. For shorter pulses, the differences in final temperature between a single pulse and 2, 3, and 6 pulses are, respectively, 24, 38, and  $65^\circ\text{C}$ . The results show a decrease of thermal confinement levels as laser pulse duration and number of pulses increases. Fractionation of laser radiation results in lower temperatures on the dentin surface and higher internal wall temperatures when compared with a single pulse radiation.

The temperature peak on surface after a single pulse of  $\tau_p=90$  ms duration was  $191^\circ\text{C}$ , approximately  $27^\circ\text{C}$  lower when compared to the shorter single pulse.

The highest temperature at the pulp wall ( $x=1.5$  mm) immediately after the end of the last pulse for both laser pulse widths was achieved using six laser pulses. Yet, while higher temperature rises at the dentin surface were observed when 0.9-ms pulses were used, there were minimal differences in the final internal wall temperature. For example the temperature differences at the pulp wall between Group 8 and Group 4 is approximately  $1.8^\circ\text{C}$ . Figures 3 and 4 show the heat distribution inside the samples, from the external surface of the dentine to the internal wall of the pulp chamber ( $x=1.5$  mm). These results represent the depth-dependent temperature calculated immediately after the end of the last pulse.

According to the results, increasing the number of pulses leads to lower temperatures at the dentin surface, while the reverse situation occurs at the pulp region. This can be due to

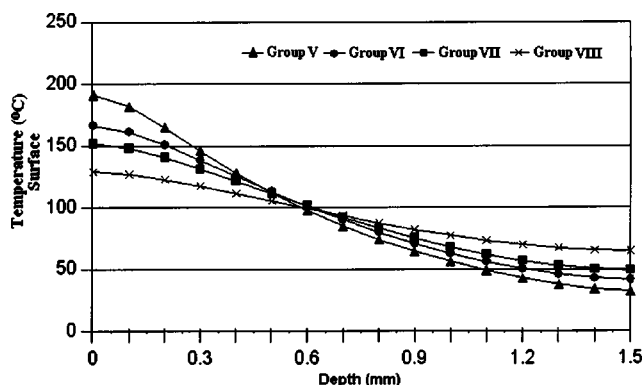


Fig. 4 Spatial temperature distribution for 1, 2, 3, and 6 pulses immediately after the end of the last laser pulse ( $\tau_p=90$  ms).

**Table 3** Final temperature immediately after Nd:YAG laser radiation at the surface and at the internal pulp wall.

	$T_{\text{surface}} (^{\circ}\text{C})$	$T_{\text{Internal Wall}} (^{\circ}\text{C}, x=1.5 \text{ mm})$
Group 1	217.9	27.2
Group 2	195.8	37.8
Group 3	179.5	45.8
Group 4	152.4	63.0
Group 5	191.0	32.2
Group 6	166.3	41.2
Group 7	151.9	49.2
Group 8	129.0	64.8

the long pulse intervals, where a sufficient period of time allows losses of energy at the surface and heat diffusion across the dentin.

The results show minimal differences in the final temperature at the internal wall after laser irradiation when the same number of pulses was used. Table 3 shows that shorter pulses result in higher temperatures at the dentin surface.

#### 4 Discussion

The photothermal interaction occurs when the molecule in the tissue absorbs luminous energy and de-excites nonradioactively producing heat. The energy absorbed by the molecule depends on the tissue composition and structure, the laser wavelength, and incident irradiance. As the tissue needs some time to conduct the heat away,<sup>20</sup> a crucial aspect in the induction of the thermal effect is the laser pulse duration. Thus, continuous wave lasers promote more evident thermal effects in the tissue when compared to pulsed lasers, even in cases where the same total energy is delivered to the tissue.<sup>21</sup>

Thermal effects in dentin surface result from photothermal interaction between tissue and laser, and occur when energy densities between 1 and  $10^3 \text{ J/cm}^2$  and exposure time between 1 s and 1  $\mu\text{s}$  are used. According LeCarpentier et al.,<sup>22</sup> pulses with typical duration of 1 ms result in higher thermal confinement than stress confinement inside the sample when compared to shorter laser pulses, yielding higher temperatures at the tissue surface.

According Van Leeween, Jansen, and Motamedi,<sup>8</sup> the thermal effects depend on laser-tissue interaction time and the resultant temperature from this process. The resultant confinement (stress or thermal) depends on the laser pulse width and the absorption coefficient of the tissue at a determined wavelength. Longer pulses mean longer interaction times between the laser and the tissue, allowing a larger diffusion of heat away from the irradiated site, and resulting in lower temperatures in the surface and higher temperatures in deeper areas. During Nd:YAG laser irradiation on dentin using short pulses ( $<1 \mu\text{s}$ ), the temperature in the radiated spot decreases during the interval between two subsequent pulses. Thus, the physical and chemical changes due to high temperatures remain

confined to a narrow region next to the surface, without much effect on deeper tissues. In general, the shorter the laser pulse, the narrower the affected region.

As seen in the results, the laser irradiation using energy fractionation of the total energy into several laser pulses leads to lower temperatures at the dentin surface; the final temperature depends on the total number of laser pulse interval and the pulse width. However, the results demonstrated that temperature accumulation on the external surface can occur during multiple-pulse irradiation, even if the pulse interval time is long (Figs. 1 and 2). On the other hand, the opposite situation occurs at the dentin internal wall, where the use of more pulses results in higher temperatures in the pulp. This can be explained by the longer pulse intervals that allow energy loss in the surface and, allow the heat diffusion toward the dental pulp.

During Nd:YAG laser irradiation, when the temperature exceeds the threshold for phase change, the ejection of a fraction of material resulting in crater formation can be observed. This ablative effect depends on the energy and duration of the laser pulse and is more evident when the tissue is exposed to long periods of exposure to the laser radiation. Therefore, significant amounts of heat can diffuse out of the area irradiated during the irradiation, reducing the local thermal damage and causing thermal damage to a larger volume of tissue.<sup>23</sup>

According to Fried et al.,<sup>17</sup> at  $\lambda = 1064 \text{ nm}$  human dentine exhibit an absorption coefficient around  $3 \text{ cm}^{-1}$  and a scattering coefficient ranging from 30 to  $200 \text{ cm}^{-1}$ . This high variation in dentine  $\mu_s$  can be explained by the differences in the density of dentin tubules. In the visible and near-infrared spectra, enamel and dentin present low absorption coefficients, thus, scattering can be considered an important parameter for determining the distribution of the energy in dentin.

Thermal effects can be associated with the thermal conduction relaxation time of tissue,<sup>20,24</sup> which is defined as the time required for the peak temperature rise ( $\Delta T_{\text{peak}}$ ) in a heated region of tissue to decrease to 37% of the total rise:

$$\tau_r = \frac{\delta^2}{N\alpha}, \quad (7)$$

where  $\delta$  is the penetration depth (cm),  $N$  is a geometric factor ( $N: 4$  to  $27$ ), and  $\alpha$  is the thermal diffusivity of the tissue ( $\text{cm}^2/\text{s}$ ).<sup>20</sup> If all the light energy is delivered in shorter pulses than the thermal relaxation time ( $\tau_p < \tau_r$ ), only a small portion of the surface will be damaged. In this case, the damage is directly proportional to the amount of energy contained in the laser pulse. However, if the interaction time is much longer than the time of thermal relaxation of the tissue ( $\tau_p > \tau_r$ ), comparatively a more evident thermal effect could be observed on the surface due to the heat dissipation toward the tissue, and consequently deeper structures of tissue can be damaged.

Since dental pulp is highly susceptible to temperature variation, even a slight rise of temperature could cause pulp cell death. Therefore, according to the simulation carried out in this work, the studied parameters are not safe for clinical procedures. However, as seen in the results, shortening the pulse width and increasing the number of pulses could avoid the thermal risk to the pulp due to the high number of pulse

intervals, even though higher total energies may be necessary to achieve the needed temperatures to induce dentin melting.

## 5 Conclusions

Optothermal simulation is important for obtaining safety parameters during laser radiation on dental hard tissue. In this work, we describe the use of a 1-D model to simulate the temperature changes in dental hard tissue during Nd:YAG laser irradiation. According to the results, the parameters studied in this work are not safe for clinical dental treatment protocols due to high temperatures resulting after Nd:YAG laser irradiation around the pulp chamber.

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